3,4-Dihydroxyacetophenone

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 43.7 L/kg

Global applicability domain: Inside

Local applicability domain index: 7.00e-01

Confidence level: 7.82e-01

Nearest Neighbors from the Training Set

Image not found
Urea, (3-methylphenyl)-
Measured: 36.3
Predicted: 37.2

Image not found
(2-Chlorophenyl)urea
Measured: 40.7
Predicted: 51.3

Image not found
N-Methyl-N'-phenylurea
Measured: 19.5
Predicted: 29.8

Image not found
3-Chlorophenylurea
Measured: 102
Predicted: 57.3